Ferromagnetic transition in a double-exchange system containing impurities in the Dynamical Mean Field Approximation

Mark Auslender[1] and Eugene Kogan[2]

[1] *Department of Electrical and Computer Engineering, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva, 84105 Israel*

[2] *Jack and Pearl Resnick Institute of Advanced Technology, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel*

(February 1, 2008)

We formulate the Dynamical Mean Field Approximation equations for the double-exchange system with quenched disorder for arbitrary relation between Hund exchange coupling and electron band width. Close to the ferromagnetic-paramagnetic transition point the DMFA equations can be reduced to the ordinary mean field equation of Curie-Weiss type. We solve the equation to find the transition temperature and present the magnetic phase diagram of the system.

PACS numbers: 75.10.Hk, 75.30.Mb, 75.30.Vn

I. INTRODUCTION

The Dynamical Mean Field Approximation (DMFA) (see [1] and references therein) is a widely used formalism for many body systems. In many cases it well takes into account non-trivial effects of strong correlations and thermal disorder. In particular, for the double-exchange (DE) model [2,3], where the exchange interaction between the core spins is mediated by mobile carriers, application of the DMFA to the description of ferromagnetic transition (see Ref. [4] and references therein) resolved a long standing problem of the energy scale for the Curie temperature T_c of manganites. However, this application was restricted to the case where only thermal magnetic disorder is present in the model. Thus, chemical disorder introduced by doping impurities, which is generic for the manganites and many other DE systems, was ignored.

It was shown however, that the concurrent action of the static and magnetic disorder is crucial for the the description of the quasi-particle and transport properties of the DE systems [5–7]. Therefore the inclusion of static disorder into the DMFA scheme is actual. The present note is devoted to this task.

II. HAMILTONIAN AND DMFA EQUATIONS

Consider the DE model with random on-site energies. The Hamiltonian of the model is

$$H = \sum_{nn'\alpha} t_{n-n'} c^\dagger_{n\alpha} c_{n\alpha} + \sum_{n\alpha} V_n c^\dagger_{n\alpha} c_{n'\alpha} - J \sum_{n\alpha\beta} \mathbf{m}_n \cdot \sigma_{\alpha\beta} c^\dagger_{n\alpha} c_{n\beta}, \quad (1)$$

where $t_{n-n'}$ is the electron hopping, V_n is the random on-site energy, J is the effective exchange coupling between a core spin and a conduction electron, $\hat\sigma$ is the vector of the Pauli matrices, and α, β are spin indices. We express the localized (classical) spin by $\mathbf{m}_n = (m_n{}^x, m_n{}^y, m_n{}^z)$ with the normalization $|\mathbf{m}|^2 = 1$.

In a single electron representation the Hamiltonian can be presented as

$$H_{nn'} = H^0_{n-n'} + (V_n - J\mathbf{m}_n \cdot \sigma)\, \delta_{nn'}; \quad (2)$$

the first is translationaly invariant, the second describes quenched disorder, and the third - annealed disorder.

The DMFA, as applied to the problem under consideration, is based on two assumptions. The first assumption is that the averaged, with respect to random orientation of localized spins and random on-site energy V, locator

$$\hat G_{\rm loc}(z) = \left\langle \hat G_{nn}(z) \right\rangle_{\mathbf{m},V}, \quad (3)$$

where

$$\hat G(z) = (z - H)^{-1}, \quad (4)$$

can be expressed through the the local self-energy $\hat\Sigma$ by the equation

$$\hat G_{\rm loc}(z) = g_0\left(z - \hat\Sigma(z)\right), \quad (5)$$

where

$$g_0(z) = \frac{1}{N}\sum_{\mathbf{k}} \left(z - H^0_{\mathbf{k}}\right)^{-1} \quad (6)$$

is the bare (in the absence of the disorder and exchange interaction) locator. Thus introduced self-energy satisfies equation

$$\hat G_{\rm loc}(z) = \left\langle \frac{1}{\hat G^{-1}_{\rm loc}(z) + \hat\Sigma(z) - V_n + J\mathbf{m}\cdot\hat\sigma} \right\rangle_{\mathbf{m},V}. \quad (7)$$

The system of equations (5) and (7) is very much similar to the well known CPA equations (see [8] and references

therein), as generalized to the case when the quantities $\hat{G}, \hat{\Sigma}$ and $\hat{g}$ are 2×2 matrices in spin space [9]. The system of equations however, is not yet closed. The averaging with respect to annealed disorder is principally different from the averaging with respect to quenched disorder.

The second assumption of the DMFA is the prescription for the determining, in our case, the probability of a spin configuration self-consistently with the solutions of the Eqs. (5) and (7). To formulate the DMFA equation for this probability, taking into account both kinds of the disorder, let us start from the general formula for the partition function

$$\mathcal{Z}_{V_n} = \int \exp\left(-\mathrm{Tr}\sum_s \log \hat{G}(z_s)\right) \prod_n d\mathbf{m}_n, \qquad (8)$$

where $z_s = i\omega_s + \mu$; ω_s is the Matsubara frequency and μ is the chemical potential. The averaging over $\{\mathbf{m}_n\}$ is given by

$$\langle \Phi \rangle_{\mathbf{m}} = \frac{1}{\mathcal{Z}_V} \int \exp\left(-\mathrm{Tr}\sum_s \log \hat{G}(z_s)\right) \Phi(\mathbf{m}) \prod_n d\mathbf{m}_n. \quad (9)$$

All observables, in particular thermodynamic potential Ω, should additionally be averaged over the realizations of the quenched disorder; in particular

$$\Omega = -\frac{1}{\beta} \langle \log \mathcal{Z}_V \rangle_{\mathbf{m},V}. \qquad (10)$$

The DMFA approximates the multi-spin probability $\mathcal{Z}_V^{-1} \exp\left(-\mathrm{Tr}\log \hat{G}\right)$ as a product of one-site probabilities in such a way, that

$$\frac{\delta \Omega}{\delta \hat{G}_{\mathrm{loc}}} = 0. \qquad (11)$$

The result for the one-site probability reads (for details of the calculation see Ref. [10]):

$$P_{V_n}(\mathbf{m}) \propto \exp\left[-\beta \Delta\Omega_{\mathbf{m},V_n}\right], \qquad (12)$$

where

$$\Delta\Omega_{\mathbf{m},V_n} = -\frac{1}{\beta}\sum_s \mathrm{Tr}\log\Big[1 + \hat{G}_{\mathrm{loc}}(z_s) \Big(J\mathbf{m}\cdot\hat{\sigma} - V_n + \hat{\Sigma}(z_s)\Big)\Big] e^{i\omega_s 0_+}. \qquad (13)$$

is the change of the thermodynamic potential of the electron gas described by the Green's function $\hat{G}_{\mathrm{loc}}$ due to interaction with a single impurity [11,12].

The right hand side of Eq. (12), is a complicated nonlinear functional of $P_V(\mathbf{m})$. However, if we are interested only in the transition temperature T_c, the problem can be reduced to a traditional mean field (MF) equation. In linear with respect to magnetization M approximation Eq. (12) takes the form

$$P_{V_n}(\mathbf{m}) \propto \exp\left(-\beta I_{V_n} \mathbf{M}\cdot\mathbf{m}\right). \qquad (14)$$

Non-trivial solution of the MF equation

$$\mathbf{M} = \int \langle P_{V_n}(\mathbf{m}) \rangle_V \, \mathbf{m} d\mathbf{m}. \qquad (15)$$

can exist only for $T < T_{\mathrm{c}}$, where $T_c = \frac{1}{3}\langle I_{V_n}\rangle_V$.

III. T_{C} FOR THE SEMI-CIRCULAR DOS

The problem of finding T_c is reduced to calculation of g_V and h_V. For simplicity consider the semi-circular (SC) bare density of states (DOS) $N_0(\varepsilon)$, the bandwidth being $2W$. Then

$$g_0(z) = \int \frac{N_0(\varepsilon)d\varepsilon}{z-\varepsilon} = \frac{2}{W}\left[\frac{z}{W} - \sqrt{\left(\frac{z}{W}\right)^2 - 1}\right]. \qquad (16)$$

For this case

$$\hat{\Sigma} = z - 2w\hat{G}_{\mathrm{loc}} - \hat{G}_{\mathrm{loc}}^{-1}, \qquad (17)$$

where $w = W^2/8$. Thus from Eqs. (5) and (7) we obtain a single equation for $\hat{G}_{\mathrm{loc}}$

$$\hat{G}_{\mathrm{loc}}(z) = \left\langle \frac{1}{z - 2w\hat{G}_{\mathrm{loc}}(z) - V_n + J\mathbf{m}\cdot\hat{\sigma}} \right\rangle_{\mathbf{m},V}, \qquad (18)$$

and Eq. (13) can be presented as

$$\Delta\Omega_{\mathbf{m},V_n} = \frac{1}{\beta}\sum_s \log\det\Big[z_s - 2w\hat{G}_{\mathrm{loc}}(z_s) - V_n + J\mathbf{m}\cdot\hat{\sigma}\Big] e^{i\omega_s 0_+}. \qquad (19)$$

In linear with respect to M approximation

$$\hat{G}_{\mathrm{loc}} = g\hat{I} - hJ\mathbf{M}\cdot\hat{\sigma}, \qquad (20)$$

where g is locator in paramagnetic phase, given by the equation

$$g = \frac{1}{2}\left[\left\langle \frac{1}{z - 2wg - V_n - J}\right\rangle_V + \left\langle \frac{1}{z - 2wg - V_n + J}\right\rangle_V\right], \qquad (21)$$

and the quantity h is given by the formula

$$h = \frac{\langle \Delta_{V_n}\rangle_V}{1 - \frac{4J^2 w}{3}\langle \Delta_{V_n}^2\rangle_V - 2w\langle \Delta_{V_n}\rangle_V}, \qquad (22)$$

where

$$\Delta_{V_n}(z_s) = \frac{1}{[z_s - 2wg(z_s) - V_n]^2 - J^2}. \qquad (23)$$

Expanding Eq. (19) we obtain the effective exchange integral is

$$I_{V_n} = \frac{4J^2 w}{\beta} \sum_s h(z_s)\Delta_{V_n}(z_s). \quad (24)$$

If we transform the sum over the imaginary Matsubara frequencies in the right-hand side of Eq. (24) to integral over real energies E, we obtain for the T_c

$$T_c = \frac{4J^2 w}{3\pi} \int_{-\infty}^{\infty} f(E)\mathrm{Im}\left[h(E_+)\left\langle \Delta_{V_n}(E_+)\right\rangle_V\right] dE, \quad (25)$$

where $f(E)$ is the Fermi function, and $E_+ = E + i0$. Eq. (25), giving the Curie temperature as a function of the parameters of the system, is the main result of the present work.

It is worth analyzing the limiting cases of this equation. In $J \gg W$ limit, shifting the energy by J, we obtain Eq. (25) in the form [13,14]

$$T_c = \frac{4w}{\pi} \int_{-\infty}^{\infty} f(E)\mathrm{Im}\left[\frac{\left\langle g_{V_n}(E_+)\right\rangle_V^2}{3 - w\left\langle g_{V_n}(E_+)^2\right\rangle_V}\right] dE, \quad (26)$$

where $g_{V_n}(E) = (E - w\left\langle g_{V_n}\right\rangle_V - V_n)^{-1}$. In the Appendix we compare the $J \ll W$ limit of Eq. (25) with the results of the Ruderman-Kittel-Kasuya-Yosida (RKKY) theory [15].

IV. PHASE DIAGRAM

Consider first the the phase diagram (PD) of the system in case of no quenched disorder. The PD is presented on Fig. 1.

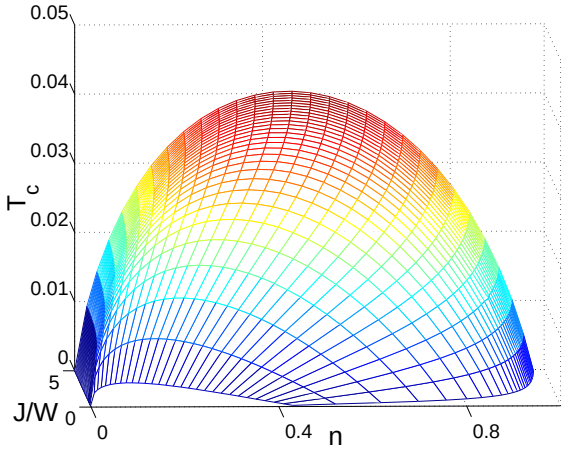

FIG. 1. The phase diagram for the case of no quenched disorder in the coordinates of relative strength of the Hund exchange J/W and electron concentration n.

In the region, where Eq. (25), gives negative value for the T_c, ferromagnetism is precluded at any temperature. From our consideration we can say nothing about the nature of the non-ferromagnetic phase (or phases), but we know from the theory of the RKKY interaction [16], that for small J/W (and no disorder), the ground state for the intermediate electron concentration is antiferromagnetic. One can say that the situation with finite Hund exchange is equivalent in some sense to the situation with the infinite Hund exchange and antiferromagnetic superexchange [17].

We consider the model of the disorder in which $V_n = V$ with the probability x, and $V_n = 0$ with the probability $1 - x$, thus x being the concentration of impurities. Solving equation for the locator for the case of strong quenched disorder ($V/W = 1$ and $x = .3$) we obtain the PD, which is presented on Fig. 2.

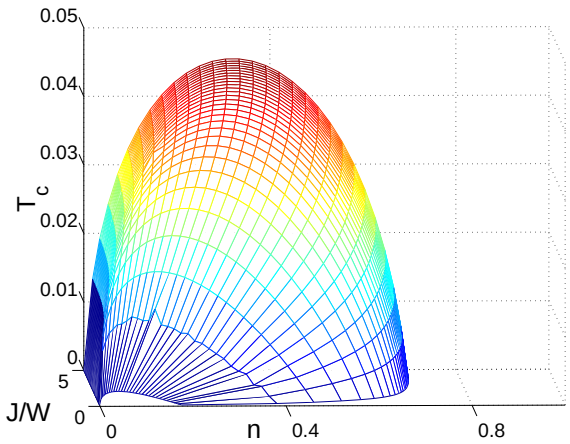

FIG. 2. The phase diagram for $V/W = 1$ and $x = .3$ in the coordinates of relative strength of the Hund exchange J/W and electron concentration n.

It is interesting that ferromagnetism is now precluded in much larger region of the $J/W - n$ plane.

This research was supported by the Israeli Science Foundation administered by the Israel Academy of Sciences and Humanities.

APPENDIX A: DMFA VS RKKY

In $J \ll W$ limit from Eq. (25) after simple algebra we obtain

$$T_c = \frac{2J^2}{3} \int_{-\infty}^{\infty} f(E)\left\{\frac{d\left\langle N_V(E)\right\rangle_V}{dE} - \frac{1}{\pi}\mathrm{Im}\left\langle g_V(E_+)^2\right\rangle_V\right\} dE, \quad (A1)$$

where $N_V(E) = -(1/\pi)\mathrm{Im}\, g_V(E_+)$ is the DOS (per one spin direction), and $g_V(E)$ is the solution of the equation

$$g_V(E) = \frac{1}{E - 2w\left\langle g_V\right\rangle_V - V}. \quad (A2)$$

In fact, in the weak exchange case we can expand Eq. (4) with respect to exchange interaction. The second order term, which is only important for us, for the diagonal matrix element of the Green's function G is

$$\hat{G}_{ll}^{(2)} = \frac{J^2}{N} \sum_{l'nn'} \frac{< ll'|nn' >}{(E-\epsilon_l)^2(E-\epsilon_{l'})} (\mathbf{m}_n \cdot \hat{\sigma})(\mathbf{m}_{n'} \cdot \hat{\sigma}), \quad \text{(A3)}$$

where

$$< ll'|nn' > \equiv \psi_l^*(n)\psi_{l'}(n)\psi_{l'}^*(n')\psi_l(n'), \quad \text{(A4)}$$

and ψ are the eigenfunctions of the non-magnetic part of the Hamiltonian: $(H_0 + V)\psi_l = \epsilon_l \psi_l$. The thermodynamic potential of the electron subsystem is given by the formula

$$\Omega^{(2)} = \frac{1}{\pi\beta} \int_{-\infty}^{+\infty} \ln\left[1 + e^{-\beta(E-\mu)}\right] \mathrm{Im} \sum_l \mathrm{Tr}\, \hat{G}_{ll}^{(2)}(E_+) dE. \quad \text{(A5)}$$

Calculating Tr with respect to spin indices and integrating by parts we obtain

$$\Omega^{(2)} = -\sum_{n \neq n'} I_{nn'} \mathbf{m}_n \cdot \mathbf{m}_{n'}, \quad \text{(A6)}$$

where

$$I_{nn'} = \frac{J^2}{\pi} \int_{-\infty}^{+\infty} f(E) \mathrm{Im} \left[\sum_{ll'} \frac{< ll'|nn' >}{(E_+ - \epsilon_l)(E_+ - \epsilon_{l'})} \right] dE. \quad \text{(A7)}$$

The exchange integral, after fulfilling in Eq. (A7) integration with respect to dE, can be presented as

$$I_{nn'} = J^2 \sum_{ll'} \frac{f(\epsilon_{l'}) - f(\epsilon_l)}{\epsilon_l - \epsilon_{l'}} < ll'|nn' > . \quad \text{(A8)}$$

To see the connection between the RKKY approximation and Eq. (A1), let us make in Eq. (A6) a mean field approximation $\mathbf{m}_n \cdot \mathbf{m}_{n'} = M^2$. Thus obtained potential can be used to construct the Landau functional of the system, which gives [14]:

$$T_c = -\frac{2}{3} \frac{\Omega^{(2)}}{NM^2}. \quad \text{(A9)}$$

Finally using the formula

$$\sum_{n \neq n'} < ll'|nn' > = \delta_{ll'} - \sum_n |\psi_l(n)|^2 |\psi_{l'}(n)|^2, \quad \text{(A10)}$$

we obtain

$$T_\mathrm{c} = \frac{2J^2}{3} \int_{-\infty}^{\infty} f(E) \left\{ \frac{dN^{(0)}(E)}{dE} - \frac{1}{\pi N} \mathrm{Im} \sum_n \left[G_{nn}^{(0)}(E_+) \right]^2 \right\} dE, \quad \text{(A11)}$$

where

$$G_{nn}^{(0)}(E) = \sum_l \frac{|\psi_l(n)|^2}{E - \epsilon_l}, \quad \text{(A12)}$$

and $N^{(0)}(E) = -(1/\pi N)\mathrm{Im} \sum_n G_{nn}^{(0)}$.

Eqs. (A1) and (A11) look very much alike. The only difference between them is ensemble averaging in Eq. (A1) vs site averaging in Eq. (A11). The DOS is self-averaging, that is $N^{(0)}(E) = \langle N_V(E) \rangle_V$, because it involves the locator itself [18]. Moreover, it is known that the CPA results for the DOS are reasonable even in the case of strong disorder. So for low electron concentration, when only the first term in Eq. (A1) (or Eq. (A11)) is important, the equations are equivalent. For higher electron concentration the term with the square of the locator decreases the T_c. According to the RKKY theory, the Curie temperature goes through zero at approximately $n = .25$ for the three principal cubic lattices [16] (for the case of no quenched disorder). Eq. (A1) for this case gives critical concentration $n = .4$. This comparison allows us to estimate the degree of agreement between the results of the DMFA and RKKY theory for the case considered. In the opposite case of very strong quenched disorder, the difference between the square of the locator in Eqs. (A1) and (A11) becomes even larger, due to the effects of localization, which are absent in the CPA. But the influence of the localization on the destruction of ferromagnetism in the DE model demands additional consideration.

[1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[2] C. Zener, Phys. Rev. **82**, 403 (1951).
[3] P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).
[4] N. Furukawa: in *Physics of Manganites*, ed. T. Kaplan and S. Mahanti (Plenum Publishing, New York, 1999).
[5] F. Zhong, J. Dong, and Z. D. Wang, Phys. Rev. B **58**, 15310 (1998).
[6] M. Auslender and E. Kogan, Eur. Phys. J. B, **19**, 525 (2001).
[7] L. P. Gor'kov and V. Z. Kresin, JETP Letters **67**, 985 (1998).
[8] J. M. Ziman, *Models of Disorder* (Cambridge University Press, Cambridge, 1979).
[9] A. Rangette, A. Yanase, and J. Kubler, Solid State Comm. **12**, 171 (1973); K. Kubo, J. Phys. Soc. Japan **36**, 32 (1974).
[10] M. Auslender and E. Kogan, Physica A **302**, 151 (2001).
[11] S. Doniach and E. H. Sondheimer, *Green's functions for solid state physicists* (Imperial College Press, London, 1998).

[12] A. Chattopadhyay, A. J. Millis, S. Das Sarma, Phys. Rev. B **61**, 10738 (2000).
[13] N. Furukawa, cond-mat/9812066.
[14] M. Auslender and E. Kogan, Phys. Rev. B **65**, 012408 (2002).
[15] J. H. Van Vleck, Rev. Mod. Phys. **34**, 681 (1962).
[16] D. C. Mattis, *The theory of magnetism*, (Springer, Berlin, 1981).
[17] J. L. Alonso, L. A. Fernandez, F. Guinea, V. Laliena, V. Martin-Mayor, cond-mat/0111244.
[18] I. M. Lifshits, S. A. Gredeskul, and L. A. Pastur, *Introduction to the theory of disordered systems* (Wiley, New York, 1988).